Ethylparaben

	-	, ,			_	
120-47	-8	D.	TX	SIE	902	2528

Model Performance

- 1		Б .
	Model	I)ata
- 1	Wiodel	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)	Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 6.59e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.25e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found

Phenylalanine

Measured: 1.34e-01 Predicted: 3.30e-01

Image not found

Phenylalanine

Measured: 1.34e-01 Predicted: 3.30e-01

Image not found

D-Phenylalanine

Measured: 1.34e-01 Predicted: 3.30e-01

Image not found

Tranexamic acid Measured: 1.06 Predicted: 1.29